

# CHEMICALS

## Project Fact Sheet



## ADVANCED AUTOTHERMAL REFORMER

### BENEFITS

- 30% to 50% reduction in  $\text{NO}_x$  emissions
- 30% to 50% reduction in  $\text{CO}_2$  emissions
- Significant energy savings resulting from up to 60% lower steam usage

### APPLICATIONS

The principal current users of synthesis gas, and hence the current market for an advanced ATR design, are the producers of ammonia and methanol. Advanced ATRs could also be used in a world-scale gas-to-liquids plant.

## REDUCING SOOT FORMATION IN AUTOTHERMAL REFORMERS COULD IMPROVE AMMONIA AND METHANOL PRODUCTION

Synthesis gas production is an intermediate step in making methanol, ammonia and oxygen-containing hydrocarbon compounds. It is a mixture of hydrogen and carbon monoxide in varying ratios depending on the desired product. The most common method used for production of synthesis gas is conventional steam reforming of natural gas. Steam reforming requires an external heat source, usually a furnace, and a nickel-based catalyst to promote the endothermic reaction. This is an energy- and capital-intensive process that produces significant  $\text{NO}_x$  and  $\text{CO}_2$  emissions.

Autothermal reforming, an energy-efficient, alternative reforming process, has been in use since the late 1950s. It uses the heat generated from combining partial oxidation and catalytic steam reformation in a single step. The technology is reliable and could significantly reduce production costs for synthesis gas. Process operating conditions must be carefully selected to minimize soot formation over a wide range of hydrogen-to-carbon ratios. Soot formation is not well understood, particularly at low steam-to-methane ratios. If the soot formation regime under a wide variety of operating conditions could be thoroughly mapped, autothermal reformers (ATRs) could replace steam-methane reformers in several industrial processes. In some applications,  $\text{NO}_x$  and  $\text{CO}_2$  emissions could be cut 30 to 50 percent over conventional reforming technology.

### ADVANCED AUTOTHERMAL REFORMER



Studies on an advanced autothermal reformer unit in Canada have provided a better understanding of the variables that define the boundaries of soot formation.



## Project Description

**Goal:** To generate a complete map of process variables which define the boundaries of soot formation in the autothermal reforming of natural gas and carbon dioxide to synthesis gas. Process variables to be studied include: feed composition, steam to hydrocarbon ratio, pressure, mixing configuration, and selection of reforming catalyst.

Elementary reaction modeling of the chemical kinetics of the gas phase partial oxidation in an ATR suggests that the presence of large amounts of CO<sub>2</sub> in the feed has only a minimal effect on the combustion characteristics. Experimental work conducted several years ago confirmed these calculations. However, the details of soot formation under these conditions, specifically high CO<sub>2</sub> recirculation, are not understood. At the temperature present in such a system it is likely that soot precursors are formed, but the rate controlling steps, including nucleation and particle growth and possible subsequent re-oxidation, cannot be quantitatively modeled at this time. As a result, to expand the market potential of this energy efficient and environmentally friendly ATR technology, direct experimental measurements of soot formation will be conducted in a small-scale reactor that permits a wide range of operating conditions to be explored.

Once the test unit is designed, built and validated, computational fluid dynamics will be used to analyze flow patterns in the test unit and scale up to commercial size. Heat and material balances will be developed for a representative size ATR using several oxidants. Flow diagrams will be developed and equipment will be sized. Process descriptions will be written and cost estimates will be developed.

## Progress & Milestones

One of the project partners, Kellogg Brown & Root, Inc., has designed and installed an ATR unit for commercial operation in Kitimat, British Columbia, Canada and recently licensed a unit in China. This latter unit will produce about 100,000 Nm<sup>3</sup>/hour of syngas. Sud Chemie continues an active program in developing new, soot-tolerant catalysts. Using CHEMKIN, a kinetics-based combustion model, initial studies on the combustibility characteristics of the system have been conducted. This preliminary work is being combined with new heterogeneous catalysis/homogeneous partial oxidation reaction modeling tools. Currently, work is progressing on the design of a test unit that will work under a wide variety of process conditions. Direct sampling and light scattering methods for soot detection and quantification are being developed.

Future research will include the following milestones:

1. Engineering, procurement and construction of the test unit
2. Validation of the burner design
3. ATR test unit operation
4. Commercial design

## Commercialization

Project partners plan to make available the commercial application of ATRs for gas-to-liquids plants within a five-year time frame. Süd Chemie will market the improved catalyst technology, while Kellogg Brown & Root will market the ATR technology.



### PROJECT PARTNERS

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